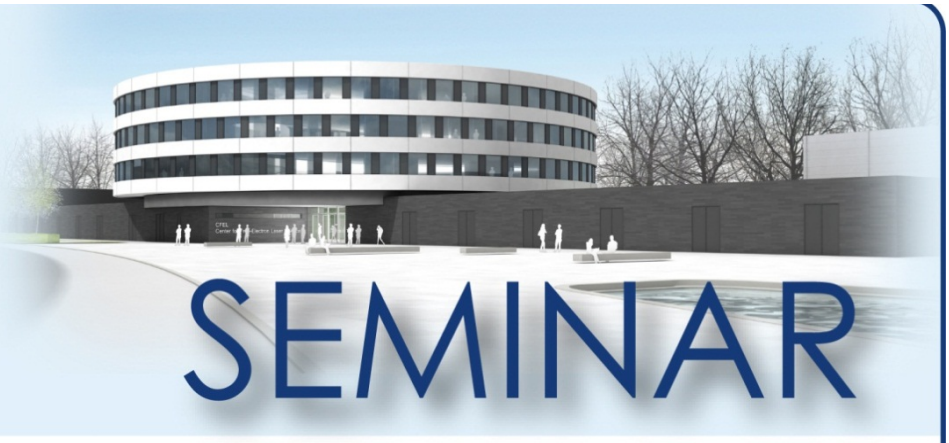
CFEL SCIENCE



SEMINAR

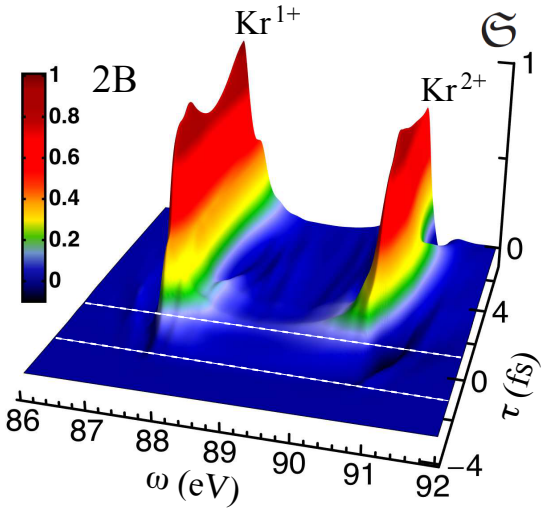
October 14, 2015 - 2:00 p.m.
CFEL-bldg. 99, seminar room IV

Gianluca Stefanucci

University of Rome Tor Vergata (Italy)

First-principles Non-Equilibrium Green's Function approach to time-resolved Photoabsorption Spectroscopy

We propose a first-principles nonequilibrium Green's function (NEGF) approach to calculate the time-resolved photoabsorption spectrum of nanoscale systems. We can deal with arbitrary shape, intensity, duration and relative delay of the pump and probe fields. We present numerical simulations of atomic systems using different approximate self-energies and, whenever possible or available, find good agreement with Configuration Interaction (CI) calculations and experiments. The NEGF approach offers a first-principle methodology to study systems are out of reach with CI and, at the same time, to include dynamical correlation effects that are difficult to describe with other methods. If time permits we will also discuss future challenges and reachable goals.



Host: Angel Rubio – MPSD-CFEL Theory Department